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1.2.2 1.2.2: Environmental transport and transformation of nanomaterials

Task Lead BOUCHARD, DERMONT
Lab/Center NERL
Division ERD
Start Date Qtr: 1 FY: 2012
End Date Qtr: 4 FY: 2016
Project 1.2: Nanomaterial-Specific Inherency Issues
Task Description
This task provides data and tools for evaluating relationships between inherent chemical properties of manufactured nanomaterials and their transport, transformation and bioavailability in environmental and treatment systems. Nanoscale metals (silver, copper/copper(II) oxide, and cerium oxide) and carbon nanotubes are included in this research. Outcomes of the research will be improved estimates of factors that affect the bioavailability of the nanometals, the persistence of carbon nanomaterials, the release of these materials from consumer products and polymer composites, and atmospheric transport of nanoscale fuel additives. The research also will lead to better predictions of the concentrations and forms of manufactured nanomaterials to which humans and ecosystems are exposed.
Research Approach
Manufactured nanomaterials are now in more than 1,300 commercial products and have found widespread applications in diverse products such as microelectronics, disinfectants in detergents, wood preservatives, nano pesticides, fillers for plastics and rubber, cosmetics/health, medical delivery devices, and construction materials, sensors, solar energy devices, image contrast agents, and various consumer products. These materials have a number of beneficial commercial uses that have resulted in increased productivity and job creation and remediation of contaminated environments. Nonetheless, the burgeoning use of nanomaterials has prompted concerns by the U.S. government about their potential (but largely unknown) impacts on human health and the environment. The U.S. EPA has been designated as one of the lead U.S. agencies in the National Nanotechnology Initiative that is evaluating these potential impacts. There are several routes that nanomaterials can be released into the environment including (1) release from household or commercial products during intended uses, (2) release from degradation of materials such as coatings of nano-metals/metal oxides or polymer nanocomposites, (3) release from combustion of fuels with nano-ceria additives; (4) discharge from wastewater treatment plants; (5) accidental spills of materials or waste streams discharged during manufacturing. As use of nanomaterials continues to escalate, the U.S. EPA will increasingly be required to assess the environmental impact of these materials. Nanomaterials pose special challenges for inherency research because tools for relating the inherent chemical properties of these materials to their transport and transformation are different from or more difficult to define, than those used for traditional chemicals. Key exposure, effects, and life cycle assessments can vary significantly along the size/surface charge/composition/dimensionality continuum of nanoparticles, which is in turn determined by complex interactions with the environment as well as in vivo systems. Developing and refining these tools are essential in meeting key program needs in risk assessment and management for a variety of carbon-based, metal oxide, and metal nanomaterials that have already been developed for use in a wide range of commercial products. Several examples illustrate the important role played by transport and transformation in evaluating exposure and risks associated with nanomaterials. In the case of nanoscale metals, the speciation of the metal is an important determinant of its biological activity. For example, in the case of Nano-Silver particles (AgNPs), Ag+ release has been shown to be the major species that causes the observed toxicity of Ag NPs. Thus, transformation of the commercial nanomaterial to its ionic form plays a key role in its exposure to human and non-human organisms. Moreover, atmospheric transport of the nanoscale cerium oxide (nanoceria) fuel additives likely plays a significant role in human exposure to this nanomaterial. Another example involves the release of nanomaterials from polymer nanocomposites which is caused primarily by photochemical transformation of the polymers. Moreover, interactions of nanomaterials such as carbon nanotubes (CNTs) with natural organic matter strongly influence both their aggregation and deposition, thus strongly affecting their transport, transformation, and exposure in aquatic environments. Of large number of nanoparticles that are currently being used, four have been identified as the short-term focus of this research effort. These nanoparticles are copper (CuNPs), AgNPs, nanoceria and CNTs. Copper and silver nanoparticles are of importance because of their strong antibacterial properties which resulted in their increasing incorporation in many consumer products such as textiles and lumber. Nanoceria is widely used as a fuel additive with little information about its environmental fate. Finally, carbon nanotubes (CNTs) exhibited some toxicological impacts that have to be evaluated in various environmental settings. It is expected that the focus of this research effort will change over the long term to address EPA□s research needs as a result of new advancements in and changes to nanomaterials applications. As a result, the focus may shift away from these nanoparticles (as more data about them is gathered) to include others that are of interest to the Agency. Examples of the research approach include: (1) developing bioavailability tools for assessing human exposures to AgNPs. This project will provide new insights into factors that influence the biological availability of these nanoparticles including the role played by manufactured coatings on the particles. A mouse model will be developed and evaluated as part of this work. Although the project primarily focuses on human bioavailability, results also should provide useful data for ecological assessments; (2) developing a high-throughput protocol for evaluating nanomaterial transport in soils and sediments. This research and development effort would build on techniques using deep well plates packed with porous media coupled with analytical plate reader methods for the rapid determination of the transport potential of microbial pathogens through sands and sediments. (3) developing and evaluating tools that describe the deposition of CNTs including effects of changing ionic and natural organic matter composition and transformations on aggregation and deposition (measured for example by attachment coefficients and critical coagulation coefficients). One goal of the projects will be to obtain data and develop relationships that that can be used in part to link ICPs of CNTs to models that predict their transport, transformation and exposure in the environment; (4) assessing emissions to the atmosphere of nano-ceria (cerium oxide) from combustion of ceria-doped fuels. This work involves characterization of the size and mixing state of ambient cerium containing particles from fuel additives based on observations and modeling. A field project in Newcastle, UK will be completed as part of the research. (5) development of data and methods for characterizing the potential leaching and availability of CuNPs from wood products to support OPP/AD regulatory decisions. This research will seek to expand the general understanding of the potential release of CuNPs from treated wood into the environment; (6) development of data and methods for characterizing metal (Ag and Cu) nanoparticles in wastewater treatment plant effluents; (7) development of methods, analyses, and reporting on the detection, evaluation and assessment of release of nanomaterials (including carbon nanotubes) from polymer composites and consumer products. The project will focus on transformations that release CNTs from their composites with polymers and also on the correlation between the mechanical and/or chemical transformation of nanomaterials from consumer products in the presence of environmental stressors and the resulting changes in inherent properties. Identification of the specific products will be in coordination with OCSPP, ILSI, and industry which will be coordinated through a CRADA to be developed.

FTE Estimates (+) (For Planning Purposes Only) [3]

Funding Estimates (+) (For Planning Purposes Only) [3]

Stakeholder Needs Met [0]

Expected Outputs (-) [5]

Description: Data on emissions produced from the use of diesel fuel containing ceria additive.
Decision/Actions:
Format: DATA
Expected Qtr: 4 **FY:** 2016

Description: Nanoparticles in the environment: Bioavailablity Assessment Tools for nanoparticles.
Decision/Actions:
Format: OTHER
Expected Qtr: 4 **FY:** 2016

Description: Transport of nanoparticles in the environment: High throughput protocols for estimating the transport of nanoparticles in environmental systems (e.g., waste water treatment plants).
Decision/Actions:
Format: OTHER
Expected Qtr: 4 **FY:** 2016

Description: Transport and transformations of nanoparticles in the environment: Experimental and modeling tools for evaluating transport and transformations of nanoparticles in the environment.
Decision/Actions:
Format: OTHER
Expected Qtr: 4 **FY:** 2016

Description: Exposure to nanoparticles in the environment: Data and relationships that can be used to link ICPs of nanoparticles to models that predict NP transport, transformation and exposure in the environment.
Decision/Actions:
Format: DATA
Expected Qtr: 4 **FY:** 2016

Expected Products (-) [17]

Description: (17) Characterization of ambient particle size distributions of ambient cerium containing particles from fuel additives using modeling.
Recipients:
Niva Kramek
Product Type: DATA
Subtype: MODEL
Delivery Date: FY2016
Date Delivered: **On Time?:** Y

Description: (14) Linkage of inherent chemical properties to nanomaterial transformation models.
Recipients:
Niva Kramek
Product Type: DATA
Subtype: MODEL
Delivery Date: FY2016
Date Delivered: **On Time?:** Y

Description: (11) Development of process models for the production of ROS by nanomaterials.
Recipients:
Niva Kramek
Product Type: DATA
Subtype: MODEL
Delivery Date: FY2014
Date Delivered: **On Time?:** Y

Description: (16) Regional scale analysis of nanoparticle transport using extended approaches that account for laboratory data developed by EPA.
Recipients:
Niva Kramek
Product Type: DATA
Subtype: SCIENTIFIC DATA
Delivery Date: FY2016
Date Delivered: **On Time?:** Y

Product Type: DATA

Description: (15) Evaluation of the influence of natural organic matter and biofilms on the transport and removal of carbon nanotubes in aqueous systems.
Recipients:
Niva Kramek
Subtype: SCIENTIFIC DATA
Delivery Date: FY2016
Date Delivered: **On Time?:** Y

Description: (12) Evaluation of emissions source terms for use in indoor air quality models that can be used to predict concentrations in realistic environments.
Recipients:
Niva Kramek
Product Type: DATA
Subtype: SCIENTIFIC DATA
Delivery Date: FY2015
Date Delivered: **On Time?:** Y

Description: (9) Evaluation of the bioavailability of Cu nanoparticles through oral and inhalation exposure routes.
Recipients:
Niva Kramek
Product Type: DATA
Subtype: SCIENTIFIC DATA
Delivery Date: FY2014
Date Delivered: **On Time?:** Y

Description: (8) Development of detection methods and data on characterize potential translocation and transformation of CNT, Ag and Cu ENPs from source to dust and other indoor surfaces.
Recipients:
Niva Kramek
Product Type: DATA
Subtype: SCIENTIFIC DATA
Delivery Date: FY2014
Date Delivered: **On Time?:** Y

Description: (6) Development of data and methods for characterizing metal (Ag and Cu) nanoparticles in wastewater treatment plant effluents.
Recipients:
Santhini Ramasamy/OW
Niva Kramek (OCSPP)
Kathleen Raffaele/OSWER
Carl Mazza/OAR
Thomas Carpenter/SAB
Product Type: DATA
Subtype: SCIENTIFIC DATA
Delivery Date: FY2014
Date Delivered: **On Time?:** Y

Description: (5) Development of data and methods for characterizing the potential leaching and availability of nano Cu/CuO from wood products.
Recipients:
Niva Kramek
Product Type: DATA
Subtype: SCIENTIFIC DATA
Delivery Date: FY2013
Date Delivered: **On Time?:** Y

Description: (13) Evaluation of Bioavailability of Micronized Copper from treated lumber.
Recipients:
Niva Kramek
Product Type: OTHER
Subtype:
Delivery Date: FY2015
Date Delivered: **On Time?:** Y

Description: (10) Development of regional scale analysis of nanoparticle transport using existing transport theory.
Recipients:
Niva Kramek
Product Type: OTHER
Subtype:
Delivery Date: FY2014
Date Delivered: **On Time?:** Y

Description: (7) Development of methods, analyses, and reporting on the detection, evaluation and assessment of release of nanomaterials (including cnts)from polymers representative of consumer products. Identification of the specific products will be in coordination with OCSPP, ILSI, industry and operate in part through a CRADA to be developed.
Recipients:
Santhini Ramasamy /OW
Niva Kramek (OCSPP)
Kathleen Raffaele/OSWER
Carl Mazza/OAR
Thomas Carpenter/SAB
Product Type: OTHER
Subtype:
Delivery Date: FY2013
Date Delivered: **On Time?:** Y

Description: (4) Assessing emissions produced from ceria doped diesel fuel.
Recipients:
Carl Mazza/OAR
Kathleen Raffaele/OSWER
Niva Kramek
Product Type: OTHER
Subtype:
Delivery Date: FY2013
Date Delivered: **On Time?:** Y

Description: (3) Evaluate and detect the deposition of carbon nanotubes on environmental surfaces.
Recipients:
Niva Kramek (OCSPP)
Kathleen Raffaele/OSWER
Carl Mazza/OAR
Thomas Carpenter/SAB
Product Type: OTHER
Subtype:
Delivery Date: FY2013
Date Delivered: **On Time?:** Y

Description: (2) Develop high throughput protocol for estimating (Ag, Cu and CNT) nanomaterial transport in soils & sediments.
Recipients:
Niva Kramek (OCSPP)
Kathleen Raffaele/OSWER
Carl Mazza/OAR
Thomas Carpenter /SAB
Product Type: OTHER
Subtype:
Delivery Date: FY2013
Date Delivered: **On Time?:** Y

Description: (1) Develop and assess bioavailability tools for assessing human exposures to silver nanoparticles.
Recipients:
Niva Kramek (OCSPP)
Kathleen Raffaele/OSWER
Carl Mazza/OAR
Thomas Carpenter/SAB
Product Type: OTHER
Subtype:
Delivery Date: FY2013
Date Delivered: **On Time?:** Y

Collaborators (+)

Milestones (-) [15]

Description: 1.1 Evaluate potential relationships between in vitro methods and preliminary in vivo assays (mouse model).
Interim Activities:
Comments:
Scheduled Qtr: 4 **FY:** 2012
Completed Qtr: **FY:**
Is this milestone on track?: Y

Description: 1.2 Determine if in vitro methods are capable of predicting results from the mouse model.
Interim Activities:
Comments:
Scheduled Qtr: 2 **FY:** 2013
Completed Qtr: **FY:**
Is this milestone on track?: Y

Description: 2.1 Refine and evaluate high throughput techniques that use deep well plates packed with porous media coupled with analytical plate reader methods for the rapid determination of the transport potential of CNT through sand/sediment.
Scheduled Qtr: 3 **FY:** 2012
Completed Qtr: **FY:**

Interim Activities:
Comments:
Is this milestone on track?: Y

Description: 3.1 Provide data and relationships for models that describe the deposition of CNTs including effects of changing ionic and natural organic matter composition on attachment coefficients and critical coagulation coefficients
Interim Activities:
Comments:
Scheduled Qtr: 4 **FY:** 2012
Completed Qtr: **FY:**
Is this milestone on track?: Y

Description: 3.2 Provide report on data and relationships that can be used to predict the effects of CNT transformations on their deposition and coagulation.
Interim Activities:
Comments:
Scheduled Qtr: 4 **FY:** 2013
Completed Qtr: **FY:**
Is this milestone on track?: Y

Description: 4.1 Provide report on the microscopic characterization of ambient (Newcastle) and freshly-exhausted cerium-containing particles from diesel fuel additives.
Interim Activities:
Comments:
Scheduled Qtr: 2 **FY:** 2013
Completed Qtr: **FY:**
Is this milestone on track?: Y

Description: 4.2 Characterize the size and mixing state of ambient cerium-containing particles from fuel additives based on observations and modeling
Interim Activities:
Comments:
Scheduled Qtr: 4 **FY:** 2013
Completed Qtr: **FY:**
Is this milestone on track?: Y

Description: 4.3 Provide report on analysis of results from a field project in Newcastle UK on transport of nanoceria from diesel fuel.
Interim Activities:
Comments:
Scheduled Qtr: 4 **FY:** 2013
Completed Qtr: **FY:**
Is this milestone on track?: Y

Description: 5.1 Development of methods for characterizing the potential leaching of nano Cu from wood products.
Interim Activities:
Comments:
Scheduled Qtr: 4 **FY:** 2012
Completed Qtr: **FY:**
Is this milestone on track?: Y

Description: 5.2 Develop and evaluate an in vitro method for the determination of the potential bioavailability of CuNP.
Interim Activities:
Comments:
Scheduled Qtr: 4 **FY:** 2013
Completed Qtr: **FY:**
Is this milestone on track?: Y

Description: 6.1 Provide data and methods for characterizing metal (Ag and Cu) nanoparticles in wastewater treatment plant effluents
Interim Activities:
Comments:
Scheduled Qtr: 4 **FY:** 2012
Completed Qtr: **FY:**
Is this milestone on track?: Y

Description: 7.1 Provide experimental and modeling tools for evaluating the effects of changing polymer nanocomposite inherent chemical properties on environmental persistence.
Interim Activities:
Comments:
Scheduled Qtr: 3 **FY:** 2012
Completed Qtr: **FY:**
Is this milestone on track?: Y

Description: 7.2 Provide report on data and relationships for polymer CNT composites that can be used to predict polymer degradation rates and accompanying CNT release.
Interim Activities:
Comments:
Scheduled Qtr: 2 **FY:** 2013
Completed Qtr: **FY:**
Is this milestone on track?: Y

Description: 7.3 Provide report documenting the changes of inherent properties of nano materials in consumer products using computational chemistry with multi-scale models characterizing activation energy, band gaps, and bonding energy.
Interim Activities:
Comments:
Scheduled Qtr: 4 **FY:** 2012
Completed Qtr: **FY:**
Is this milestone on track?: Y

Description: 7.4 Provide report on the correlation between the mechanical and/or chemical transformation of nanomaterials from consumer products in the presence of environmental stressors and the resulting changes in inherent properties.
Interim Activities:
Comments:
Scheduled Qtr: 4 **FY:** 2013
Completed Qtr: **FY:**
Is this milestone on track?: Y

Facilities Needed [0]

Categories (+) [1]

Suggestions/Feedback?